MATERIALS SCIENCES DIVISION

03-01

Magnetism at the Atomic Scale

Interactions of Single Atoms and Pairs of Atoms Studied

Direct studies of the properties of single magnetic atoms and pairs of magnetic atoms have been made by atomic scale imaging using a specially built scanning tunneling microscope (STM). The single atom studies confirm theoretical predictions regarding the interaction of magnetic atoms with the surface of a metal in the so-called Kondo regime. The studies of pairs of atoms reveal that "Kondo molecules" can be formed. This work of LBNL scientists Michael Crommie and Steven Louie extends fundamental research on the details of magnetism to the atomic scale.

Familiar magnetic phenomena such as ferromagnetism (permanent magnets) are due to the collective behavior of the "magnetic moments" of unpaired electrons in materials such as certain transition metals (Fe, Cr, etc.). It is of fundamental interest in condensed matter physics, as well as in technologies such as information storage, to learn how these collective behaviors scale down to atomic dimensions. Also, because any future magnetic nanotechnologies will require that small magnetic entities be in contact with other materials, it is of interest to understand the interaction of small groups of magnetic atoms with different environments, such as a metal surface.

Recent advances in scanning probe microscopies have enabled the detailed study of properties of surfaces and surface adsorbates with true atomic-scale resolution (see MSD Highlights 02-2 and 00-8). These types of studies have provided critical tests of predicted behavior and have uncovered new phenomena. Here, an atomic resolution STM was employed to study the properties of small groups of magnetic atoms on the surface of a conducting metal. It was discovered in the 1960's through the study of the electrical resistance of dilute solutions of magnetic atoms in metals, that, at cryogenic temperatures, the magnetic moments of the atoms can interact with the free electrons of the metal to form a new coupled state that is characterized by a "Kondo resonance." To study this effect on the atomic scale, the LBNL researchers placed single atoms of a magnetic atom (Ti) on the surface of a metal (Ag) and observed the electronic structure of the atom with the STM tip at 6.8 K. They measured the density of filled states by causing electrons to "tunnel" out of the atom with a negative sample bias and the density of empty states by causing electrons to "tunnel" into the atom with a positive sample bias. By suitable data processing, it was possible to separate the two contributors to the data: the characteristic Kondo resonance of the Ti single atom and the so-called d-resonance (see figure). The broadening of the shape of the Kondo resonance voltage differences between minimum and maximum points (see figure) as the temperature was increased to 49 K was measured; the behavior was in agreement with a theoretical prediction that had not previously been experimentally confirmed.

Next, the team studied the Kondo behavior of pairs of Ni atoms, forming Ni₂ "molecules" by pushing them together with the STM tip. In this way, the characteristic parameters of the Kondo interaction could be measured as a near-continuous function of interatomic distance. It was found that the observations could be explained by the formation of an Ni₂ "Kondo molecule" at interatomic distances smaller than 4 Angstroms. This assignment was supported by *ab initio* calculations performed by the Louie group.

These fundamental studies of the behavior of atomic-scaled magnetic systems represent critical tests of the limits of understanding of magnetism in condensed matter physics.

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